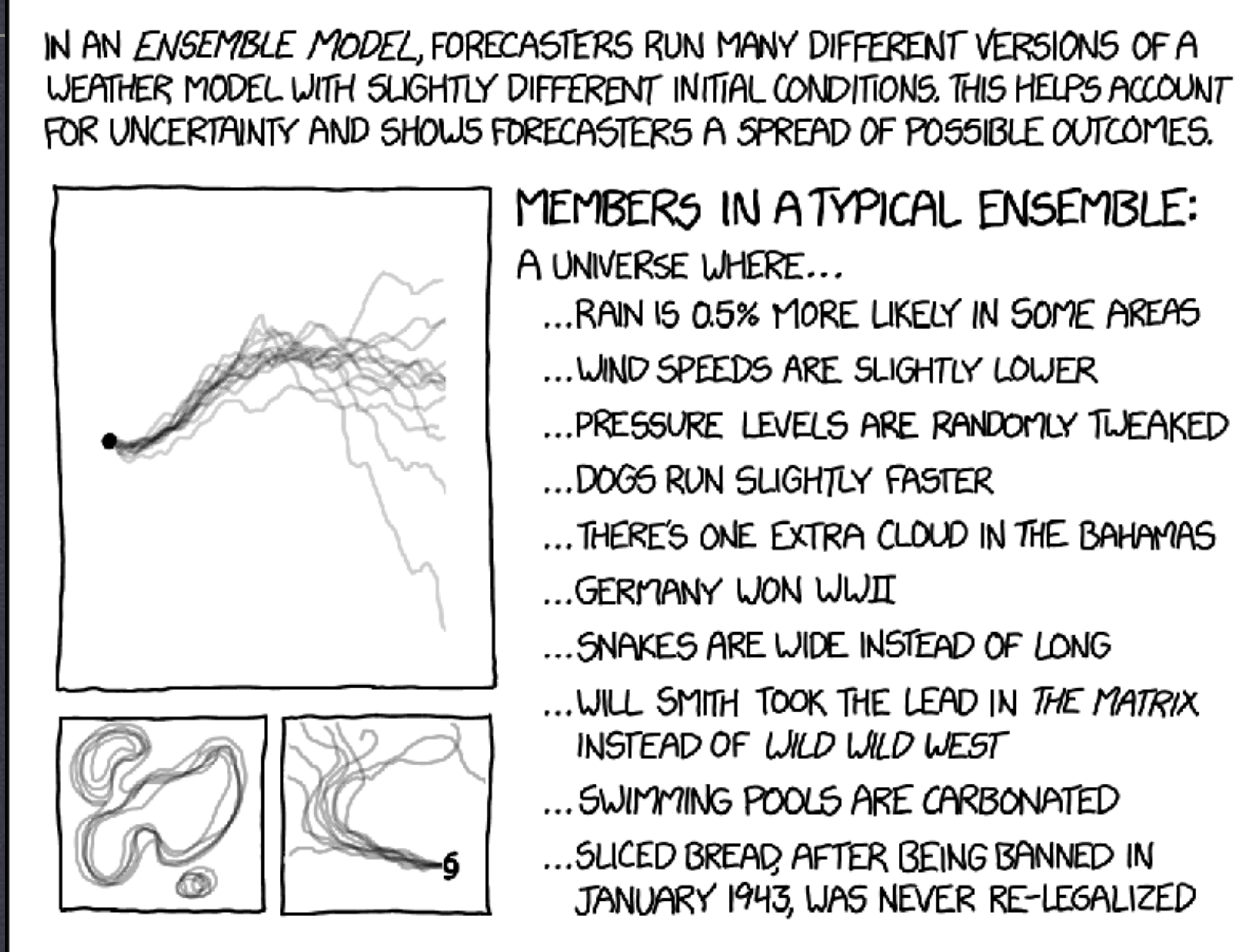
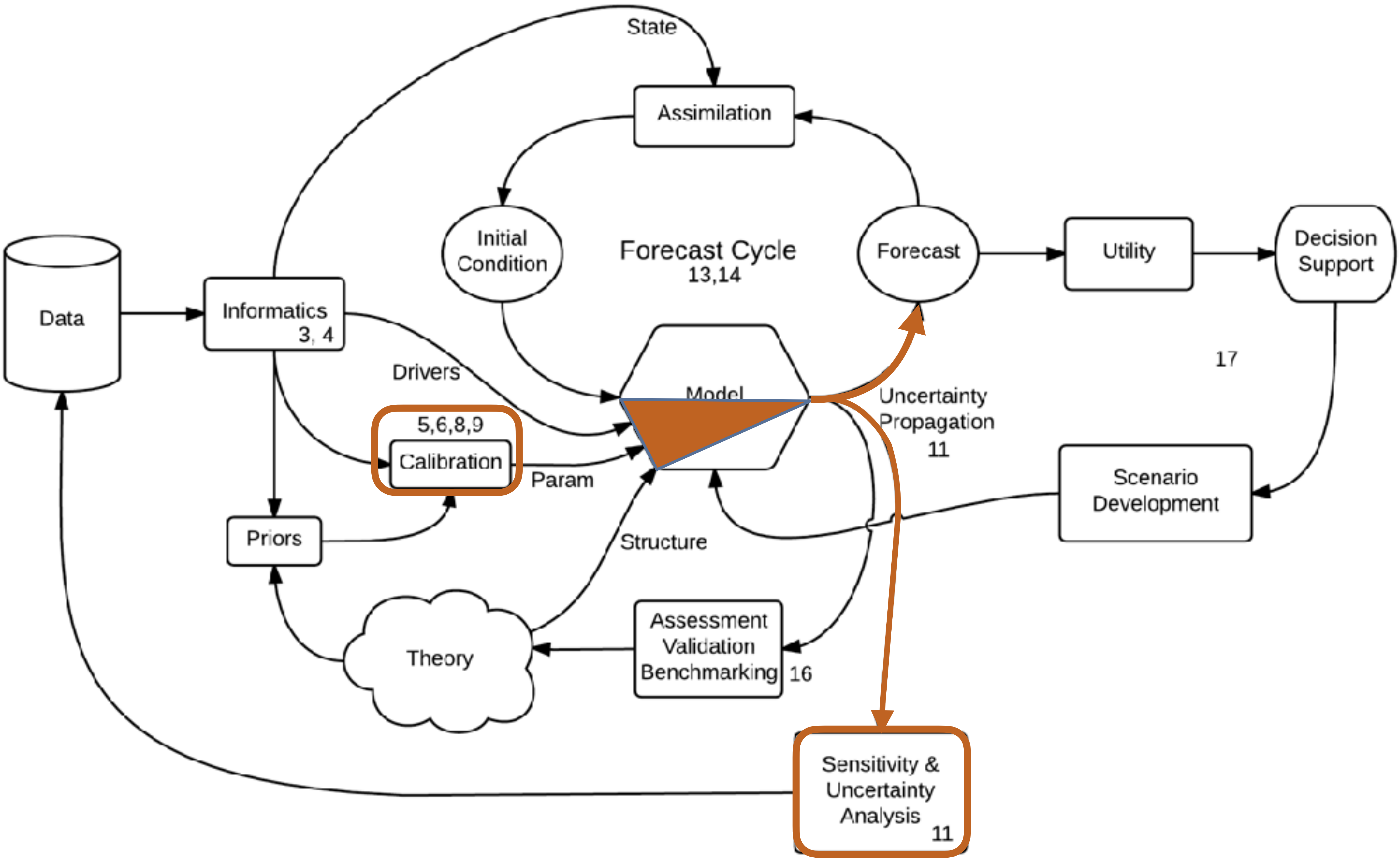


PROPAGATING, ANALYZING, AND REDUCING UNCERTAINTY


State
Assimilation
Initial Condition
Forecast Cycle
13,14
Forecast
Utility
Decision Support
Data
Informatics
3, 4
Drivers
Model
5,6,8,9
Calibration
Param
Uncertainty Propagation
11
17
Scenario Development
Priors
Structure
Assessment Validation Benchmarking
16
Theory
Sensitivity & Uncertainty Analysis
11

Concepts

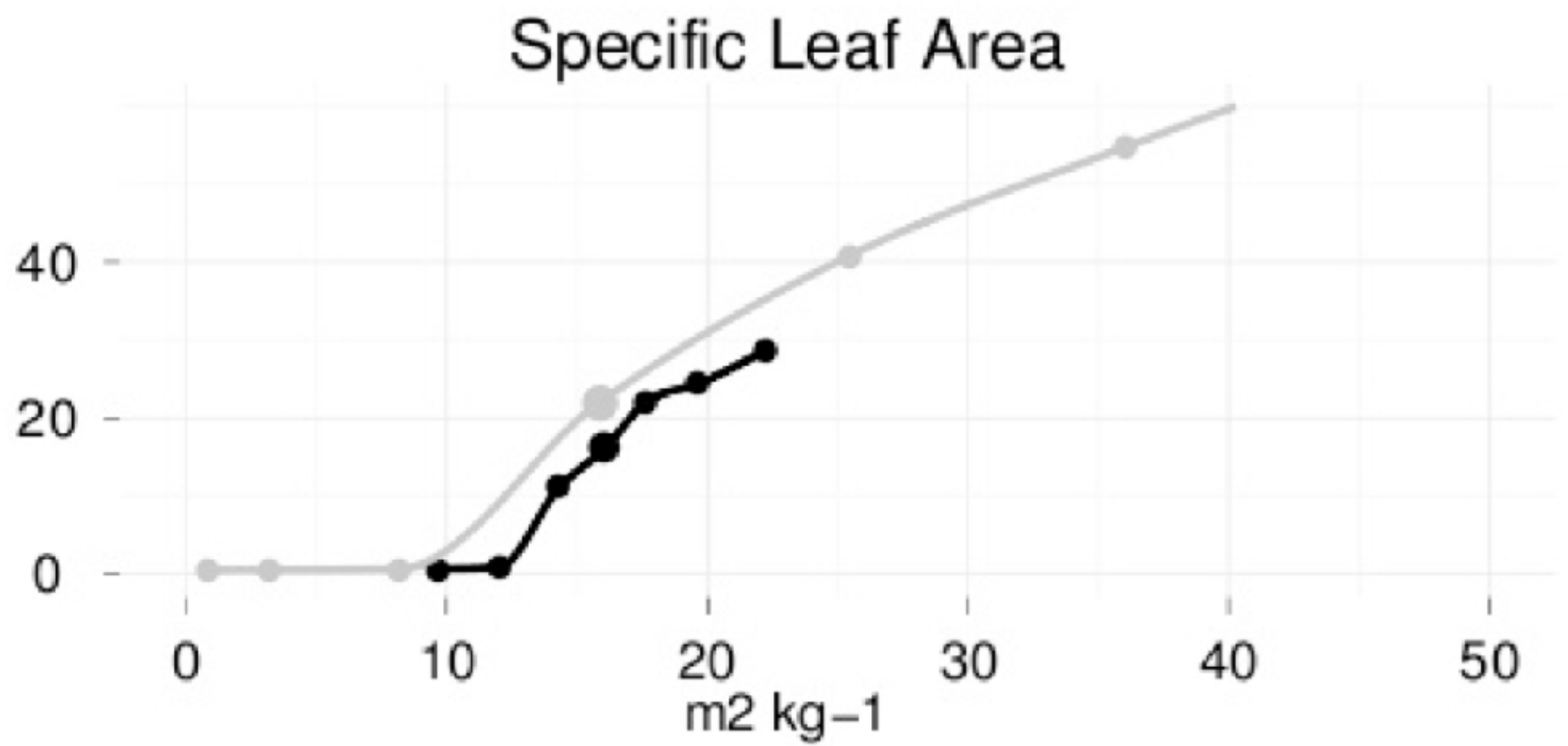
- Sensitivity Analysis
  How does a change in X translate into a change in Y?
- Uncertainty Propagation
  How do we forecast Y with uncertainty?
  How does the uncertainty in X affect the uncertainty in Y?
- Uncertainty Analysis
  which sources of uncertainty are most important?
- Optimal Design
  How do we best reduce the uncertainty in our forecast?

Sensitivity Methods

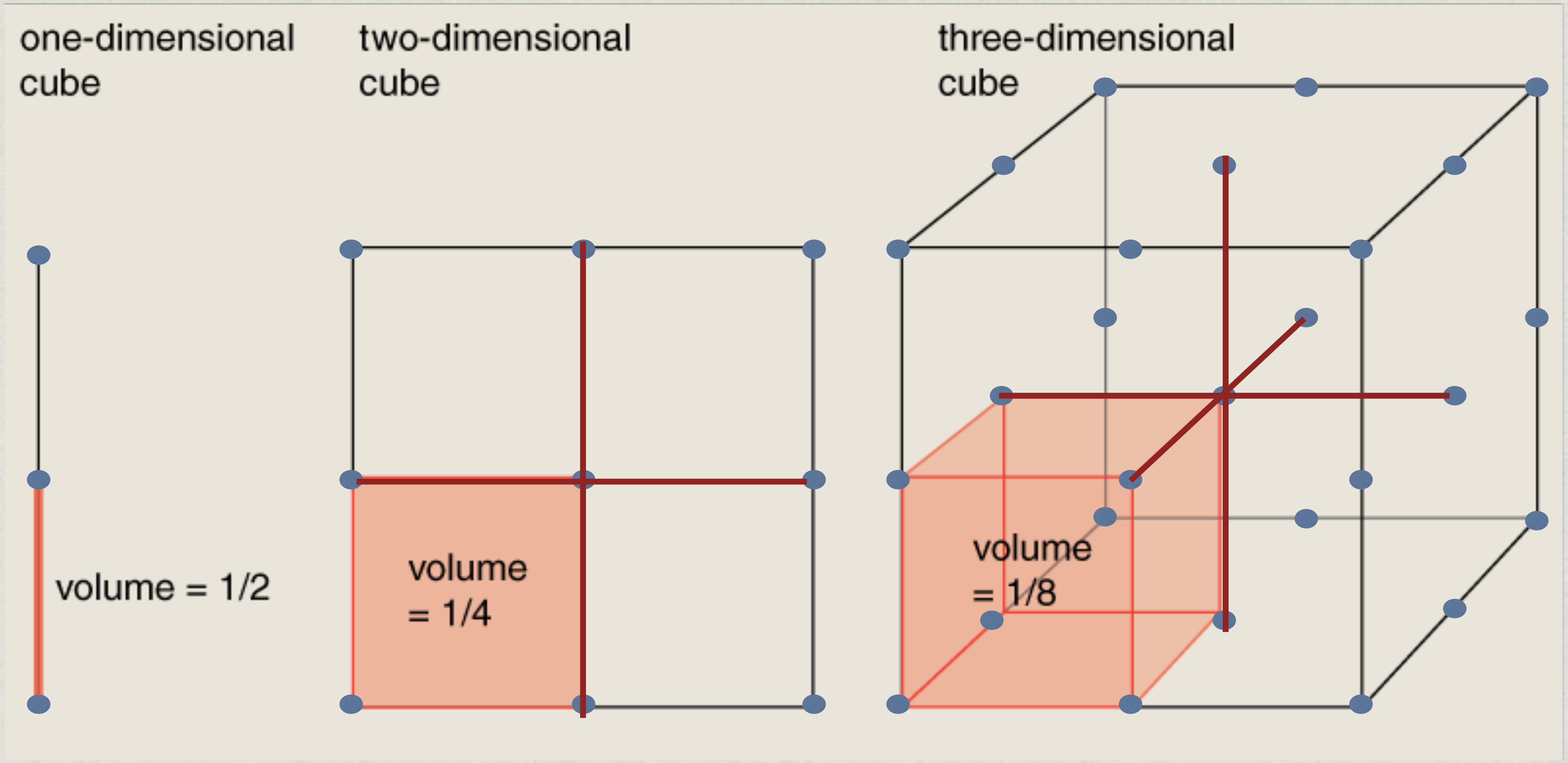
- Local
  - Analytical: $df/d\Theta$
  - One-at-a-time perturbations

Saltelli et al. 2008. Global Sensitivity Analysis

Sensitivity Analysis



Global Sensitivity



Curse of Dimensionality

Sensitivity Methods

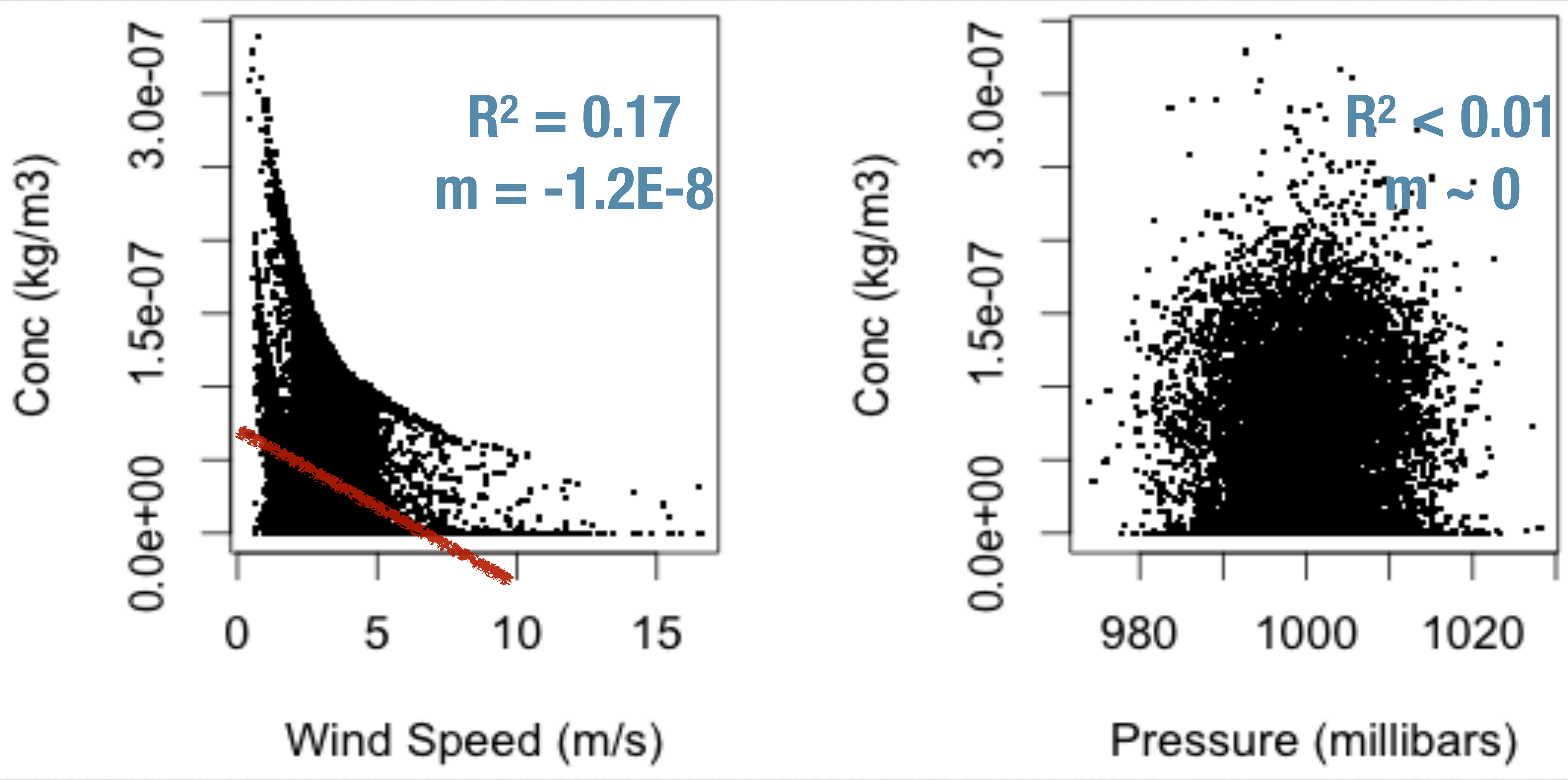
- Local
  - Analytical: $df/d\Theta$
  - One-at-a-time perturbations
- Global
  - Monte Carlo
  - Sobol
  - Emulators
  - Elementary Effects
  - Group Sampling

Extensive but Costly

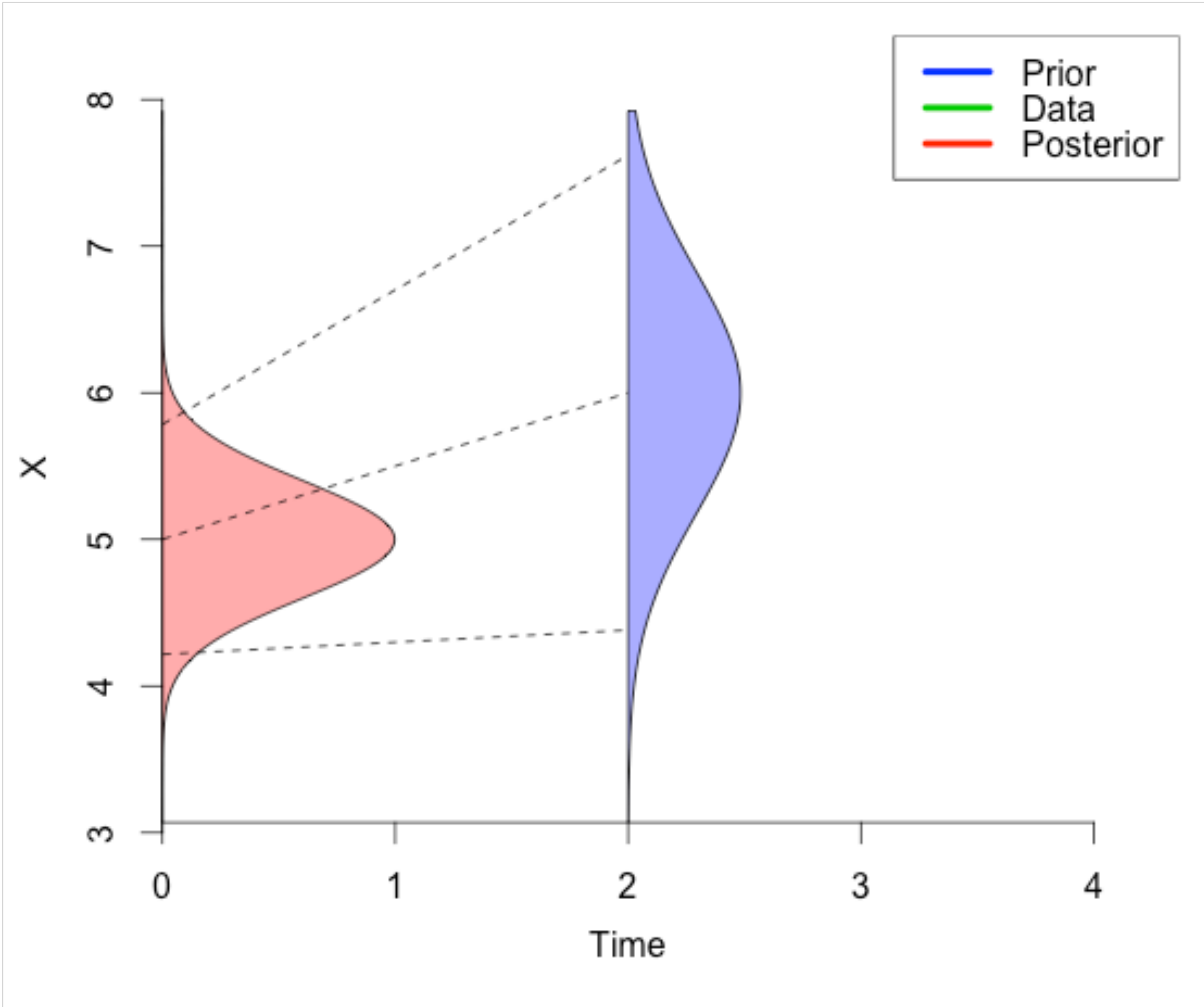
Sparse but Cheap

Saltelli et al. 2008. Global Sensitivity Analysis

Monte Carlo Sensitivity

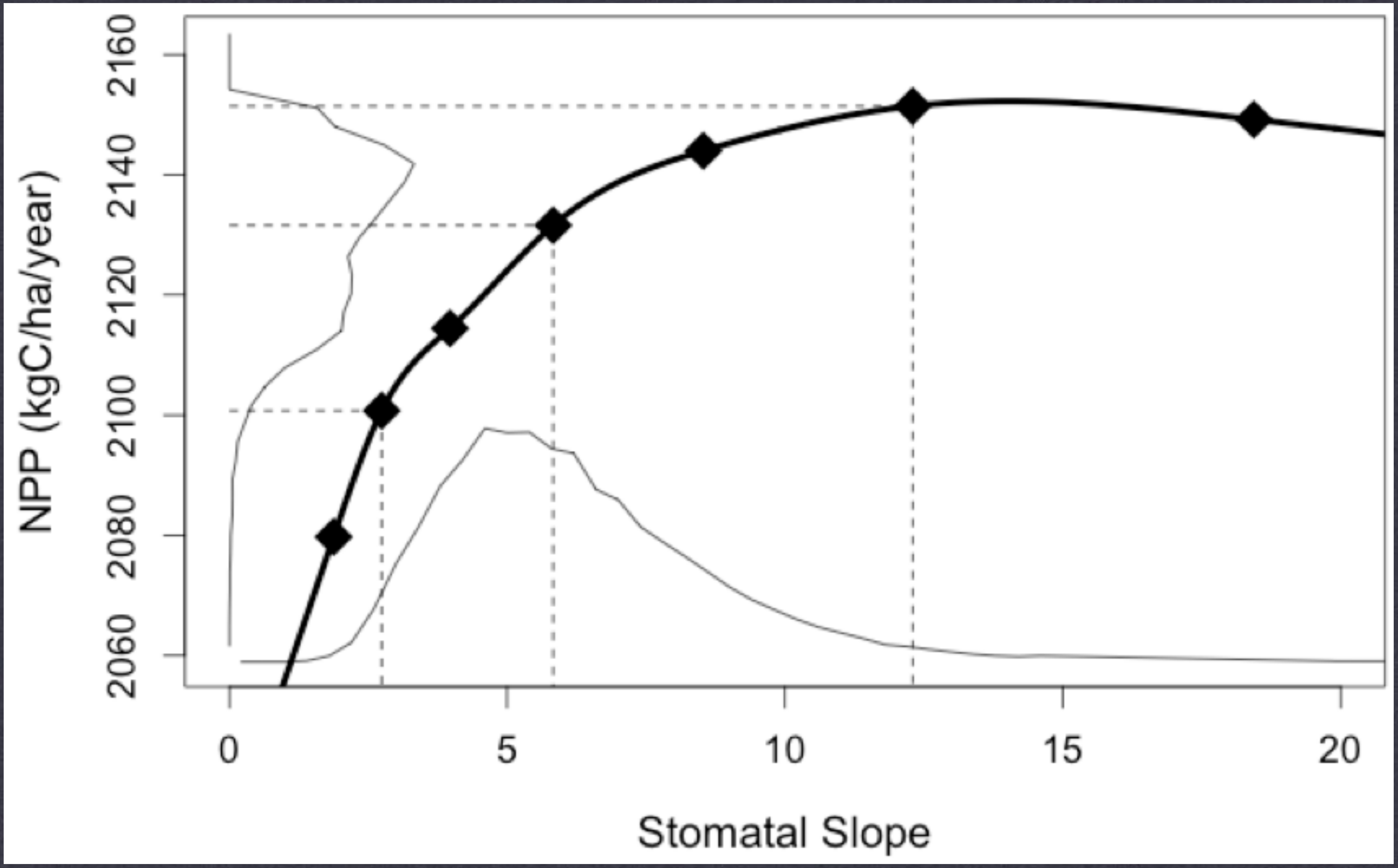


Free if you do MC uncertainty propagation or MCMC



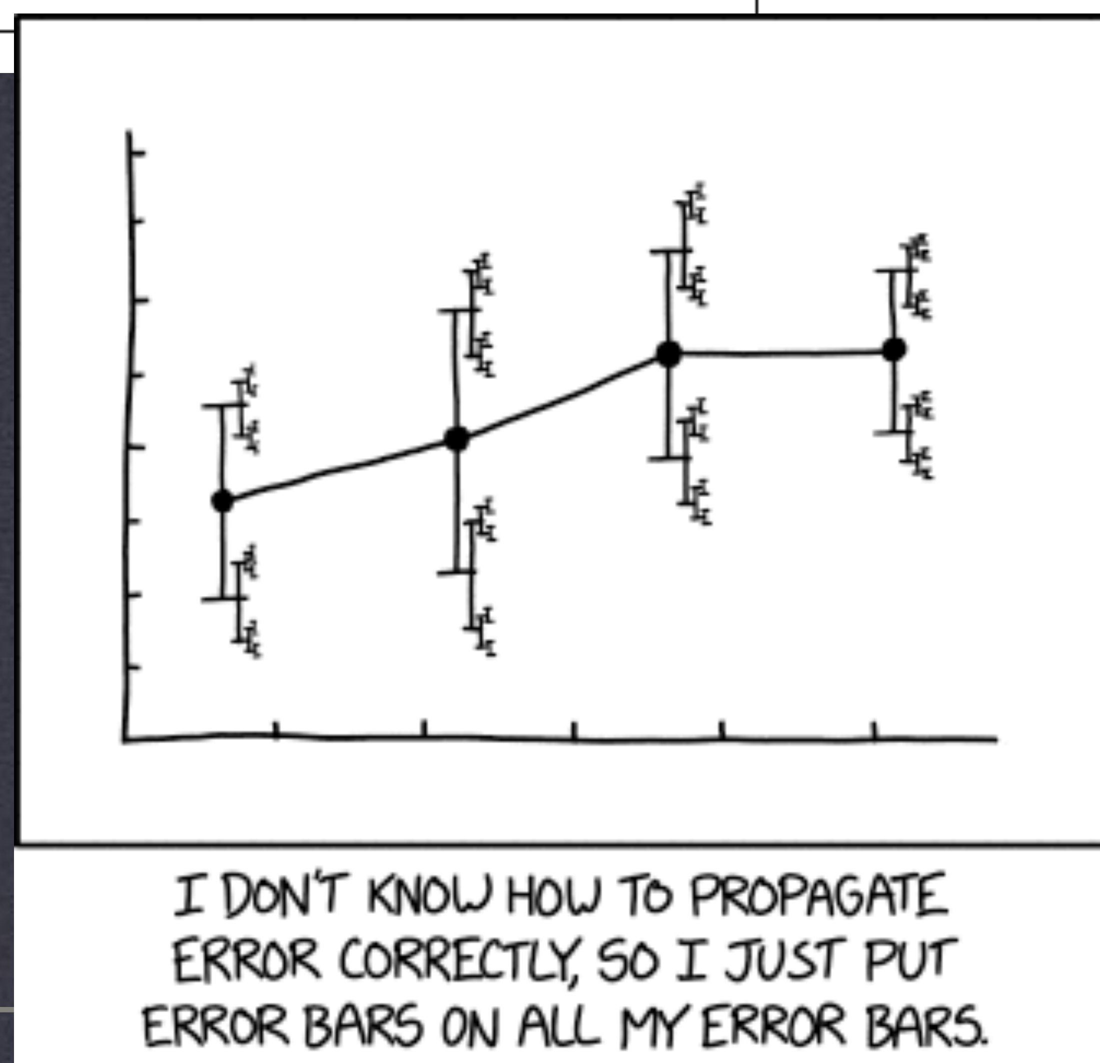
Prior
Data
Posterior
X
8
7
6
5
4
3
0
1
2
3
4
Time

UNCERTAINTY PROPAGATION



UNCERTAINTY PROPAGATION

Approach		Output: Distribution	Output: Moments
	Analytic	Variable Transform	Analytical Moments Taylor Series
	Numeric	Monte Carlo	Ensemble



VARIABLE TRANSFORM

$$P_Y[y] = P_\theta[f^{-1}(y)] \cdot \left| \frac{d\, f^{-1}(y)}{dy} \right|$$

Analytical Moments

$$Var(aX) = a^2 Var(X)$$

$$Var(X + b) = Var(X)$$

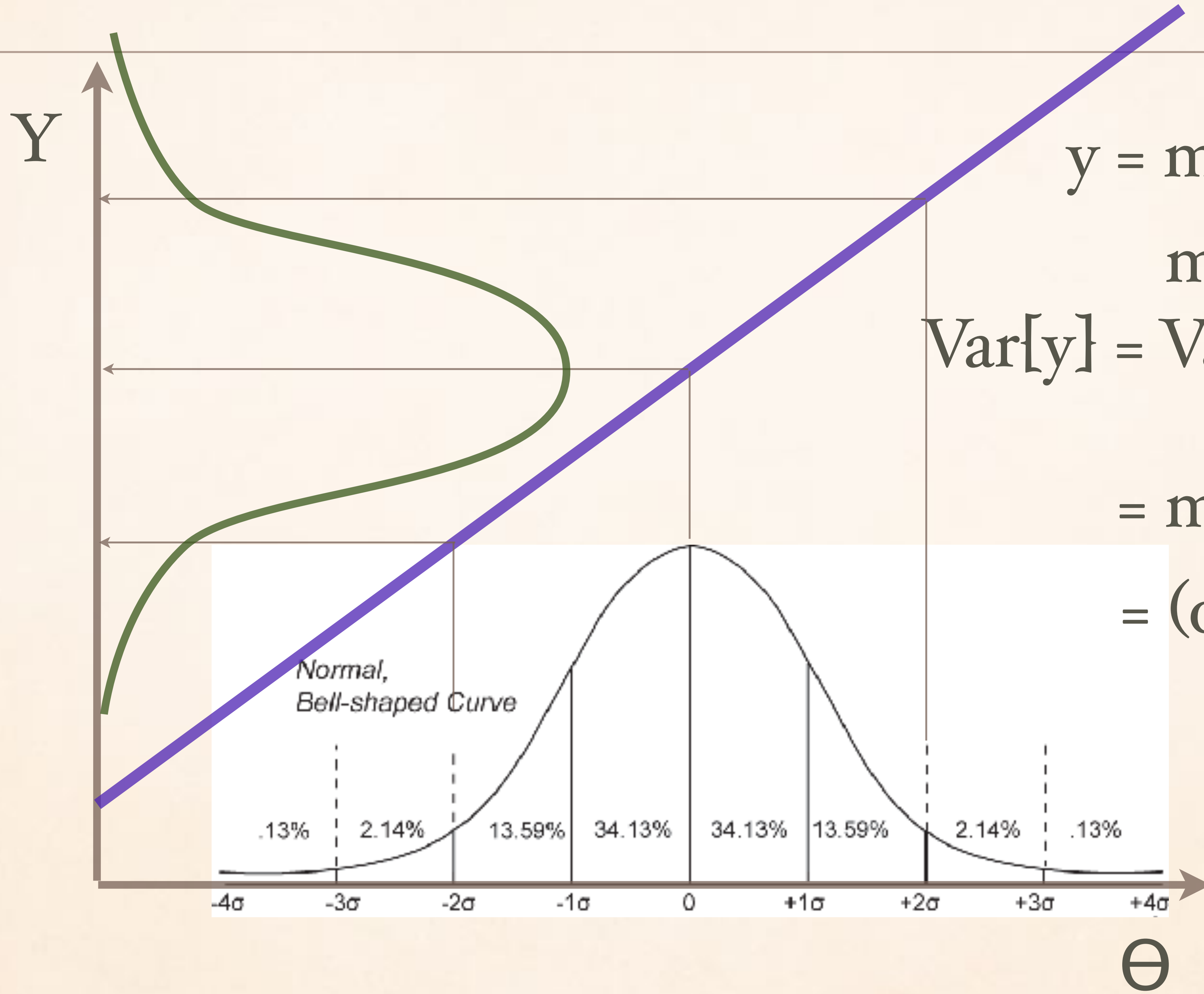
$$Var(X + Y) = Var(X) + Var(Y) + 2\mathrm{Cov}(X, Y)$$

$$Var(aX + bY) = a^2 Var(X) + b^2 Var(Y) + 2\mathrm{abCov}(X, Y)$$

$$Var\left(\sum X\right) = \sum Var(X_i) + 2\sum_{i<j} Cov(X_i, X_j)$$

$$Var(X) = Var(E[X|Y]) + E[Var(X|Y)]$$

REL'N TO SENSITIVITY



$$y = m\Theta + b$$

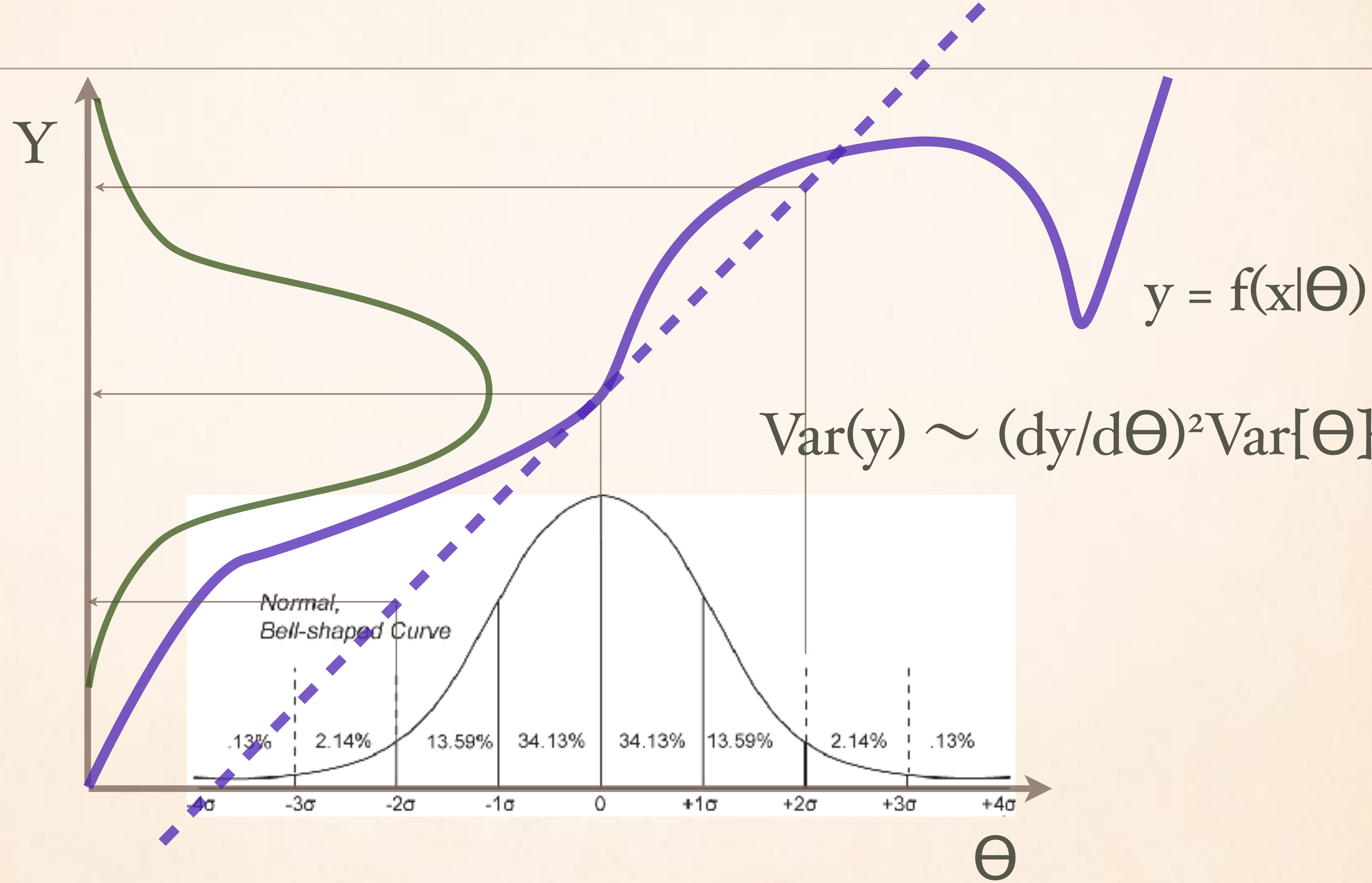
$$m = dy/d\Theta$$

$$\mathrm{Var}\{y\} = \mathrm{Var}[m\Theta + b\}$$

$$= m^2\mathrm{Var}[\Theta]$$

$$= (dy/d\Theta)^2\mathrm{Var}[\Theta\}$$

TAYLOR SERIES



LINEAR APPROX

$$Var[f(x|\theta)] \approx Var\left[f(x|\bar{\theta}) + \frac{\frac{df}{d\theta}(x|\bar{\theta})}{1!}(\theta - \bar{\theta}) + \ldots \right]$$

$$var[f(x)] \approx \left(\frac{\partial f}{\partial \theta_i} \right)^2 var[\theta]$$

LINEAR APPROX

$$Var[f(x|\theta)] \approx Var\left[f(x|\bar{\theta}) + \frac{\frac{df}{d\theta}(x|\bar{\theta})}{1!}(\theta - \bar{\theta}) + \ldots \right]$$

$$var[f(x)] \approx \sum \left(\frac{\partial f}{\partial \theta_i} \right)^2 var[\theta_i] +$$

$$\sum_{i \neq j} \left(\frac{\partial f}{\partial \theta_i} \right) \left(\frac{\partial f}{\partial \theta_j} \right) cov[\theta_i, \theta_j]$$

$$Y_{t+1} = f(Y_t, X_t | \theta) + \varepsilon$$

$$Var[Y_{t+1}] \approx \underbrace{\left(\frac{df}{dY}\right)^2}_{stability} \underbrace{Var[Y_t]}_{\substack{IC \\ uncert}} + \underbrace{\left(\frac{df}{dX}\right)^2}_{\substack{driver \\ sens}} \underbrace{Var[X]}_{\substack{driver \\ uncert}} + \underbrace{\left(\frac{df}{d\theta}\right)^2}_{\substack{param \\ sens}} \underbrace{Var[\theta]}_{\substack{param \\ uncert}} + \underbrace{Var[\varepsilon]}_{\substack{process \\ error}}$$

COV & SCALING

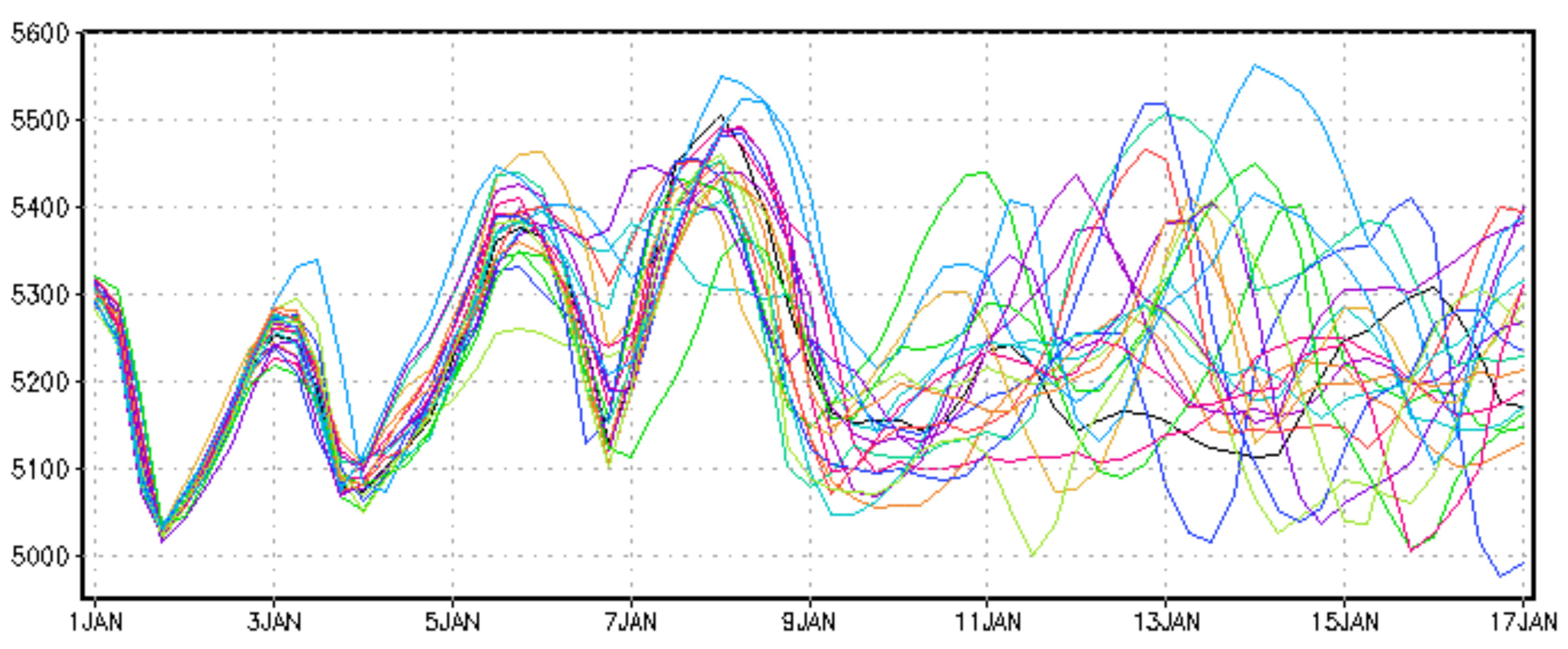
- **Scaling very dependent on spatial and temporal auto- & cross-correlation**

$$\sum\sum\frac{\partial f}{\partial X_i}\frac{\partial f}{\partial X_j}COV[X_i, X_j]$$

UNCERTAINTY PROPAGATION

		Output	
		Distribution	Moments
Approach	Analytic	Variable Transform	Analytical Moments Taylor Series
	Numeric	Monte Carlo	Ensemble

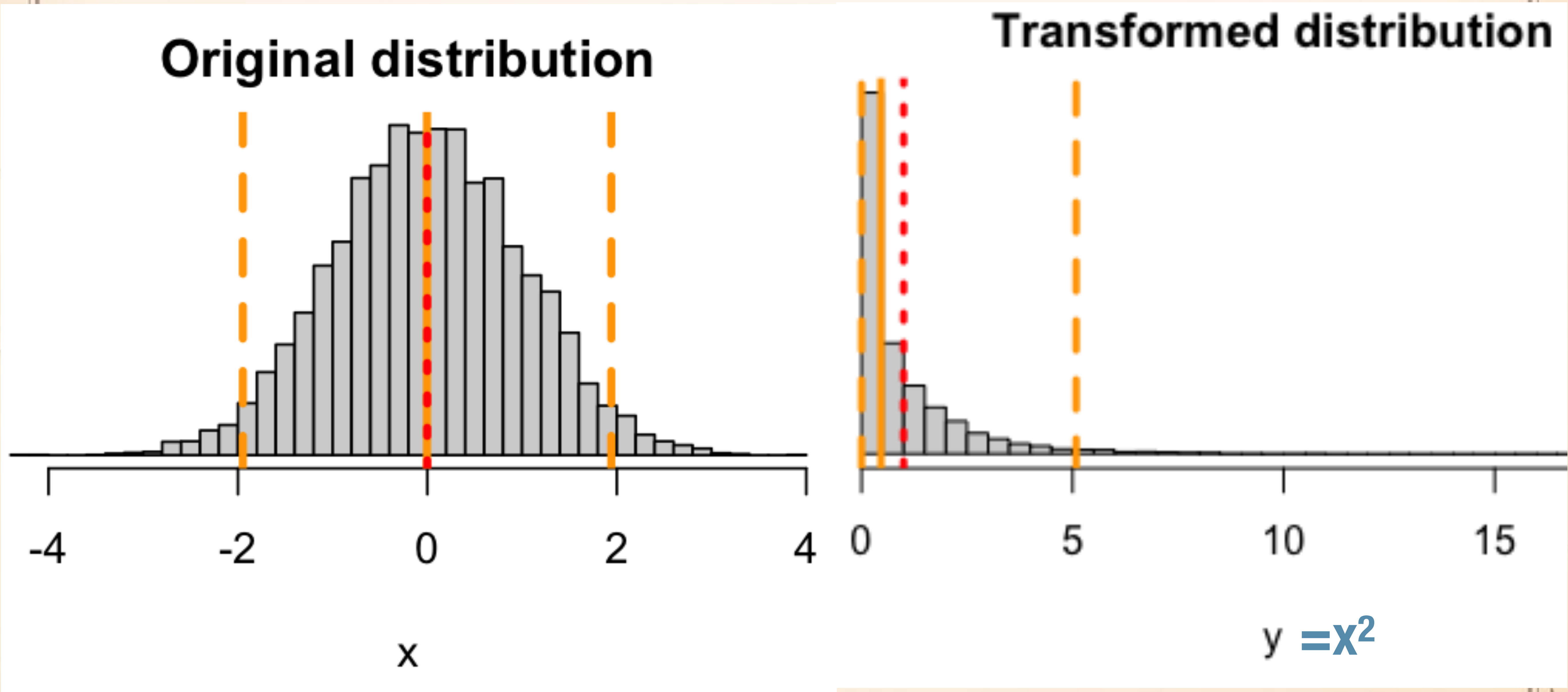
Numerical Approximation



- Monte Carlo Simulation --> Distribution
- Ensemble Analysis --> Moments

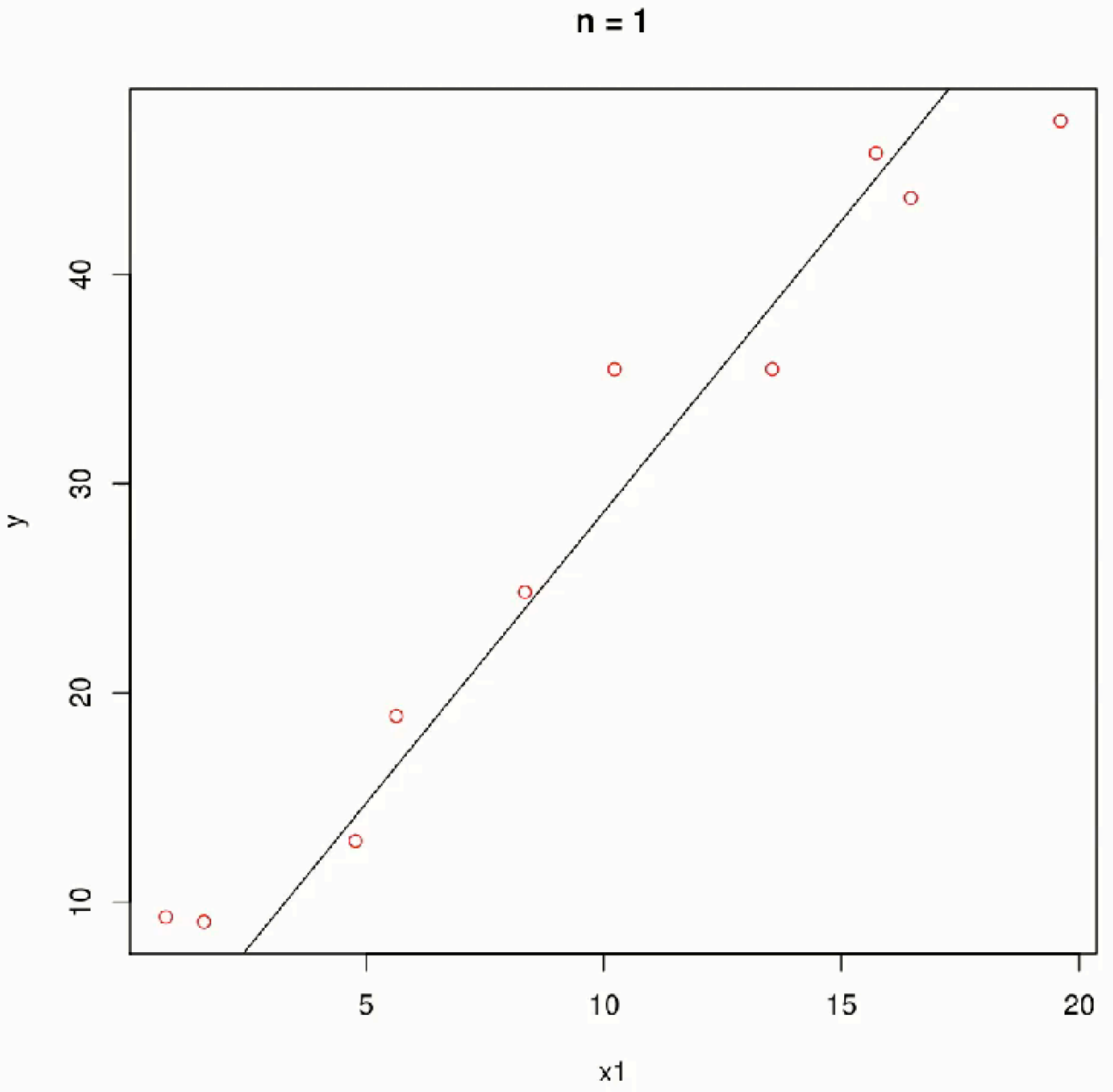
JENSEN'S INEQUALITY

$$f(\bar{x}) \neq \overline{f(x)}$$



MONTE CARLO UNCERTAINTY

- for (i in 1:n)
  - draw random values from distributions
  - run model
  - save results
- summarize distributions

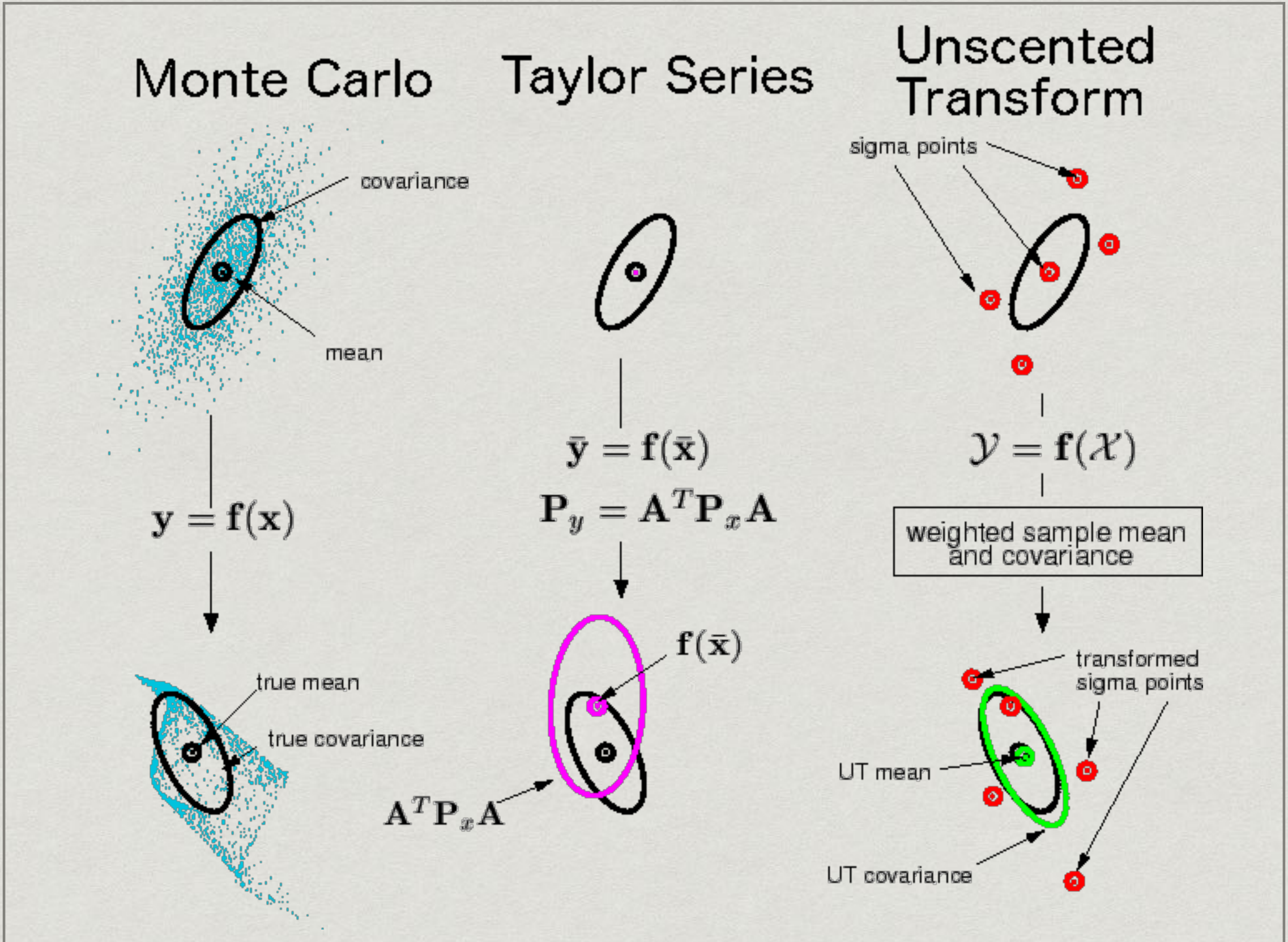

n = 1
y
10
20
30
40
5
10
15
20
x1

ENSEMBLE UNCERTAINTY

- for (i in 1:n)
  - draw random values from distributions
  - run model
  - save results
- **Fit PDF to results**
- **Use PDF for intervals, etc.**

Requires smaller N to estimate moments than to approximate full PDF

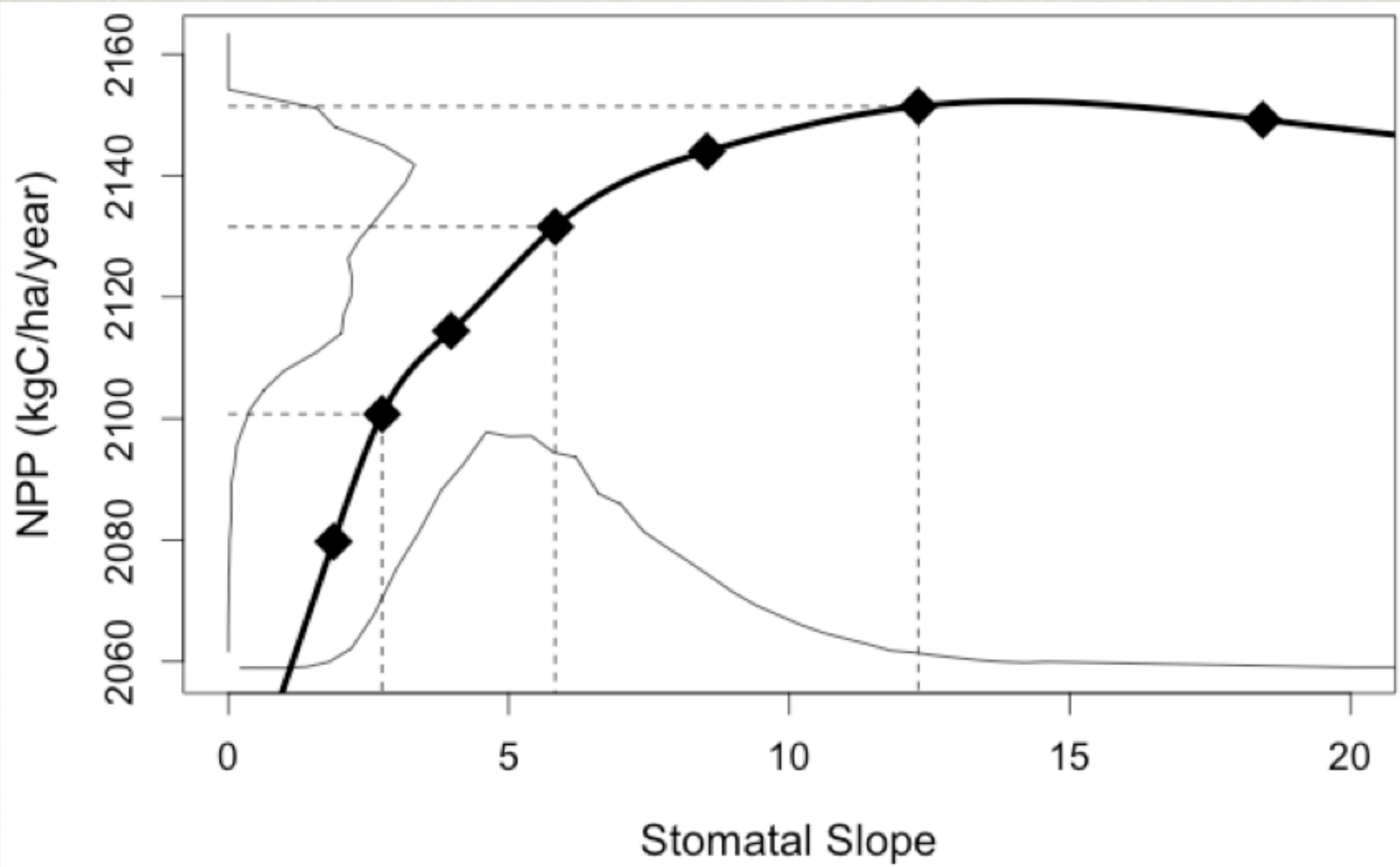
Already have this from MCMC!

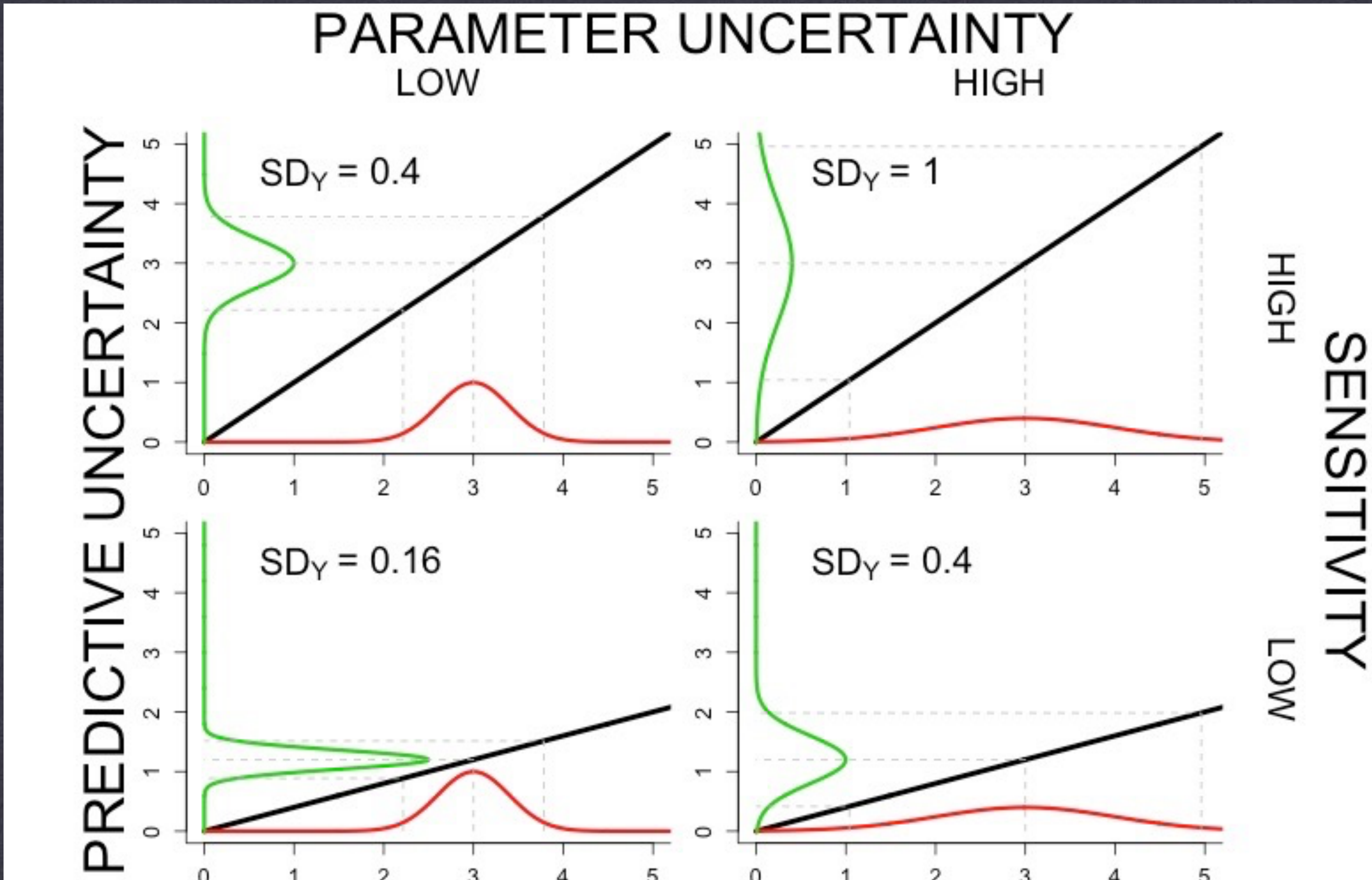

Monte Carlo
Taylor Series
Unscented Transform
covariance
mean
$\mathbf{y} = \mathbf{f}(\mathbf{x})$
true mean
true covariance
$\bar{\mathbf{y}} = \mathbf{f}(\bar{\mathbf{x}})$
$\mathbf{P}_y = \mathbf{A}^T\mathbf{P}_x\mathbf{A}$
$\mathbf{f}(\bar{\mathbf{x}})$
$\mathbf{A}^T\mathbf{P}_x\mathbf{A}$
sigma points
$\mathcal{Y} = \mathbf{f}(\mathcal{X})$
weighted sample mean and covariance
transformed sigma points
UT mean
UT covariance

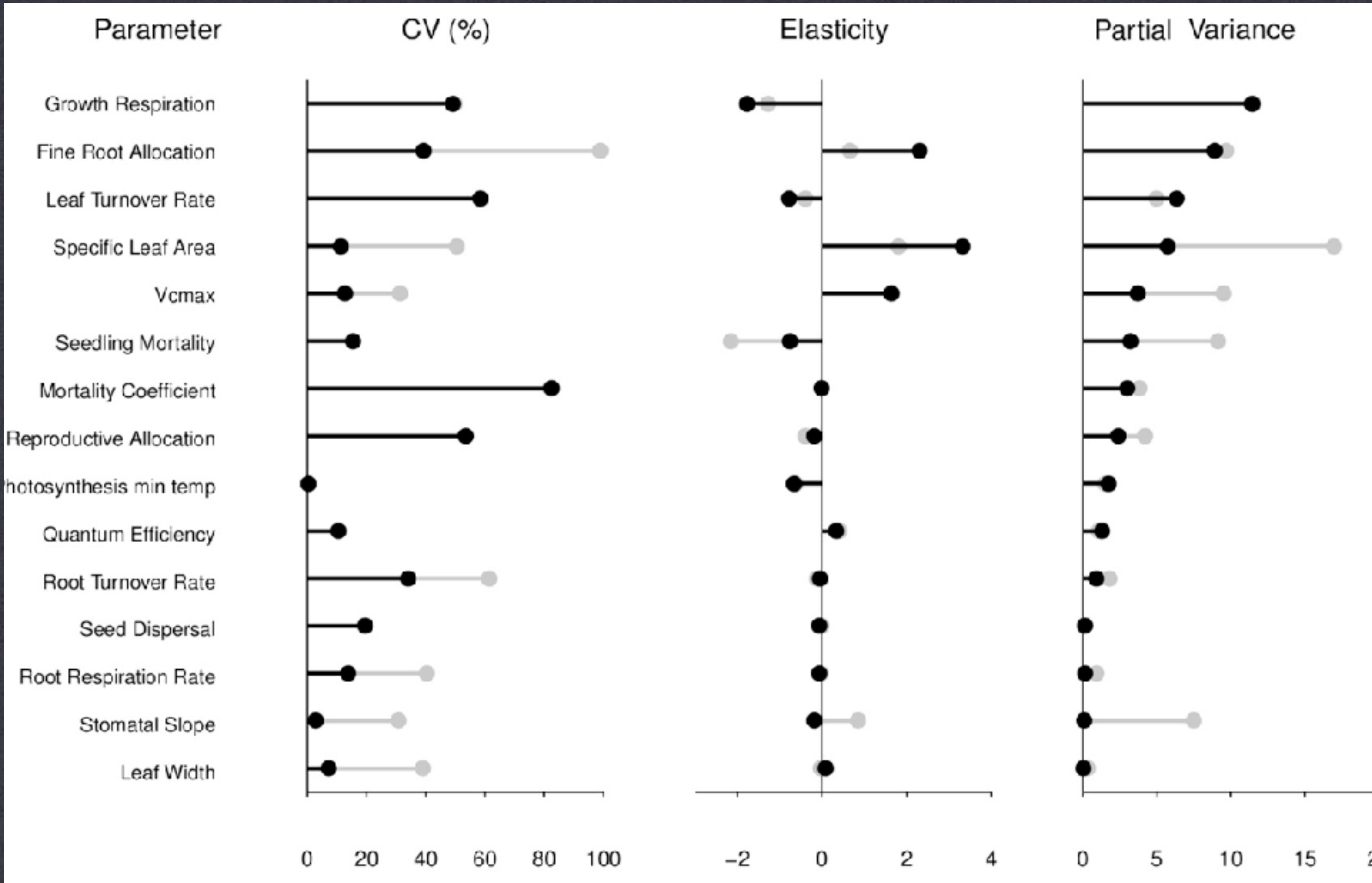
UNCERTAINTY PROPAGATION

		Output	
		Distribution	Moments
Approach	Analytic	Variable Transform	Analytical Moments Taylor Series
	Numeric	Monte Carlo	Ensemble

Uncertainty Analysis



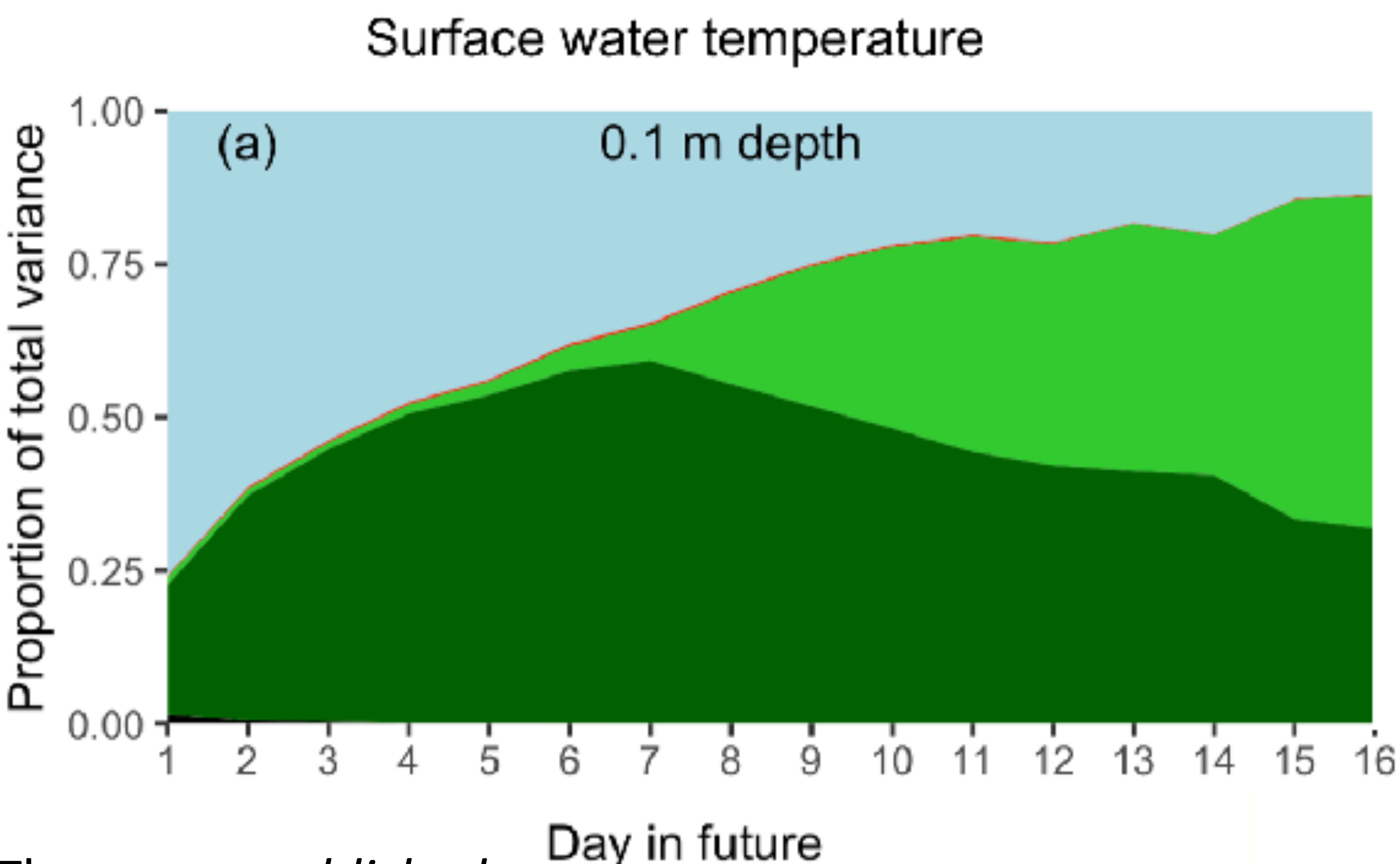

PARAMETER UNCERTAINTY
LOW
HIGH
PREDICTIVE UNCERTAINTY
SENSITIVITY
HIGH
LOW
$SD_Y = 0.4$
$SD_Y = 1$
$SD_Y = 0.16$
$SD_Y = 0.4$



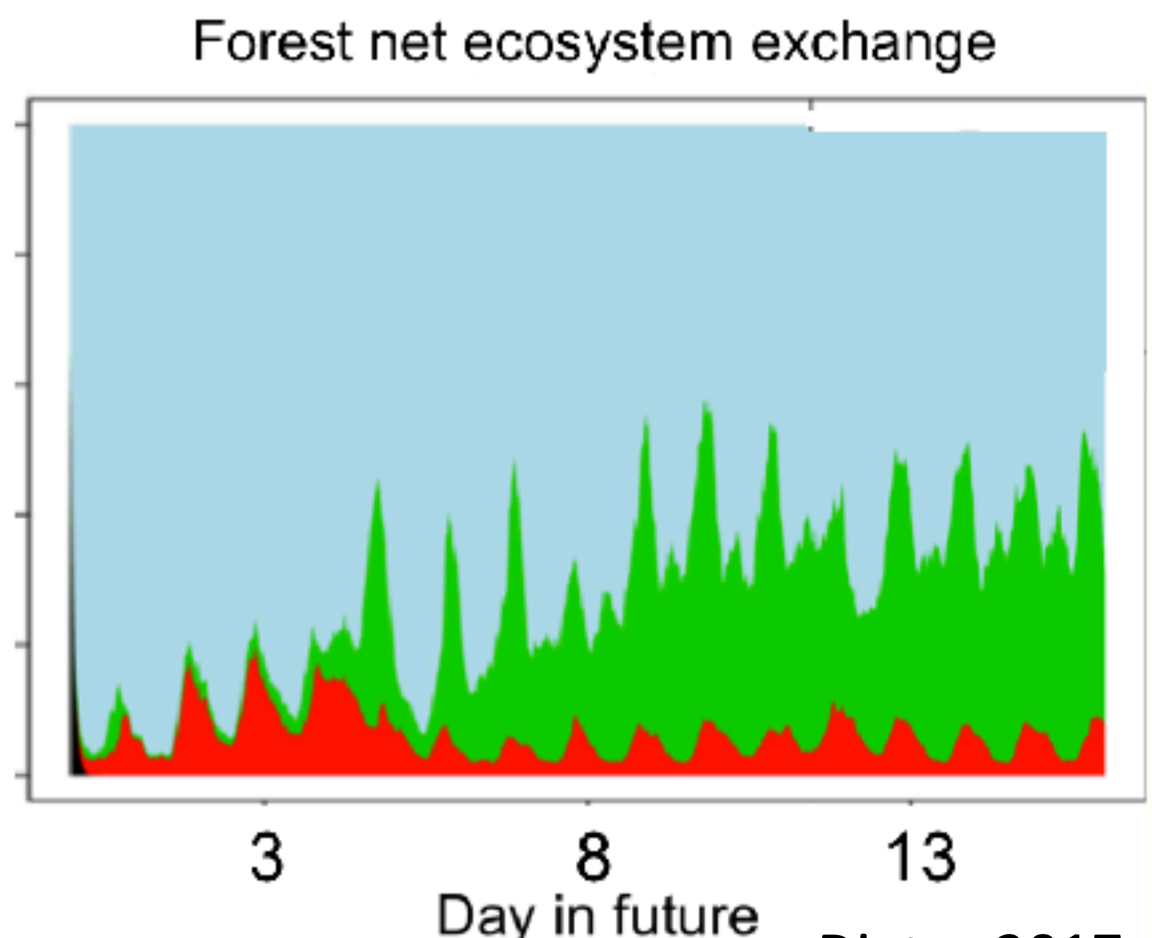
VARIANCE DECOMPOSITION

SWITCHGRASS YIELD, CENTRAL ILLINOIS

How do the drivers of forecast uncertainty vary across ecological system?



Thomas *unpublished*



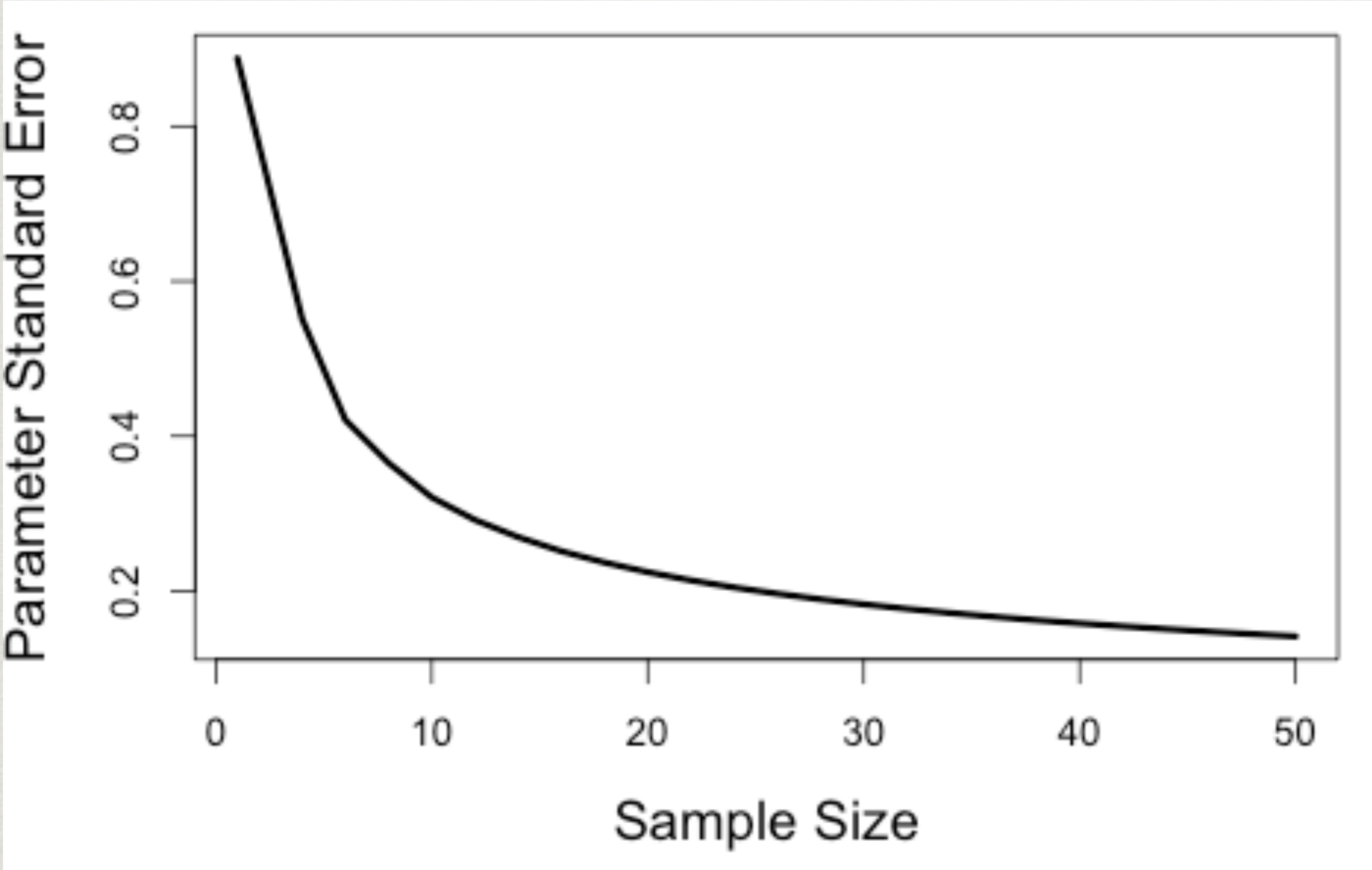
Dietze 2017

UNCERTAINTY: driver: meteorology; driver: meteorology downscaling; initial conditions (IC); parameter; process

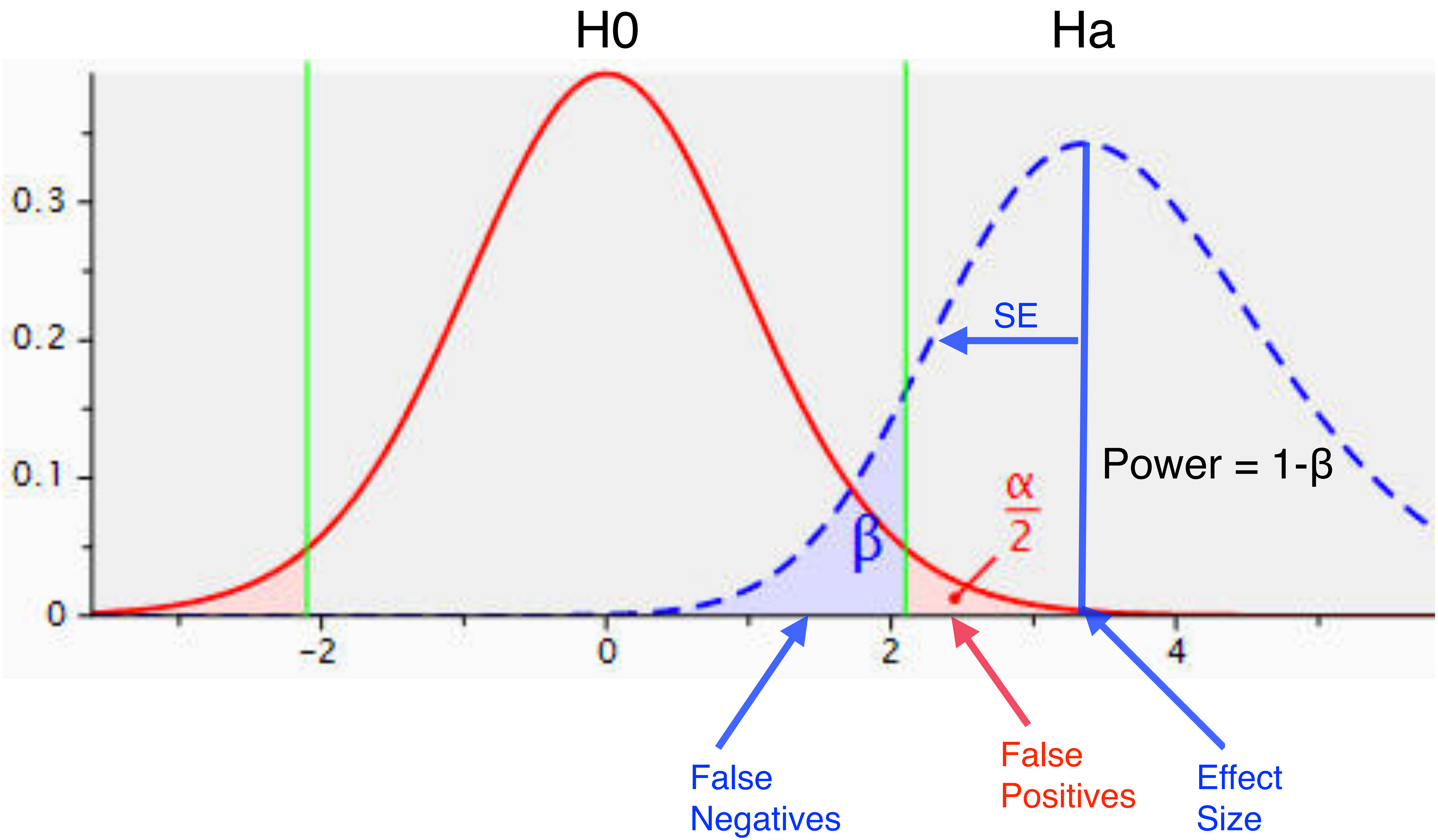
Tools for model-data feedbacks

- **Power analysis**
  - Sample size needed to detect an effect size
  - Minimum effect size detectable given a size
- **Observational design**
  - What do I need to measure?
  - Where should I collect new data?
  - How do I gain new info most efficiently?

SE ∝ 1/sqrt(n)



Parameter Standard Error
0.2
0.4
0.6
0.8
0
10
20
30
40
50
Sample Size



Power = f(effect size, SE)

Pseudo-data simulation

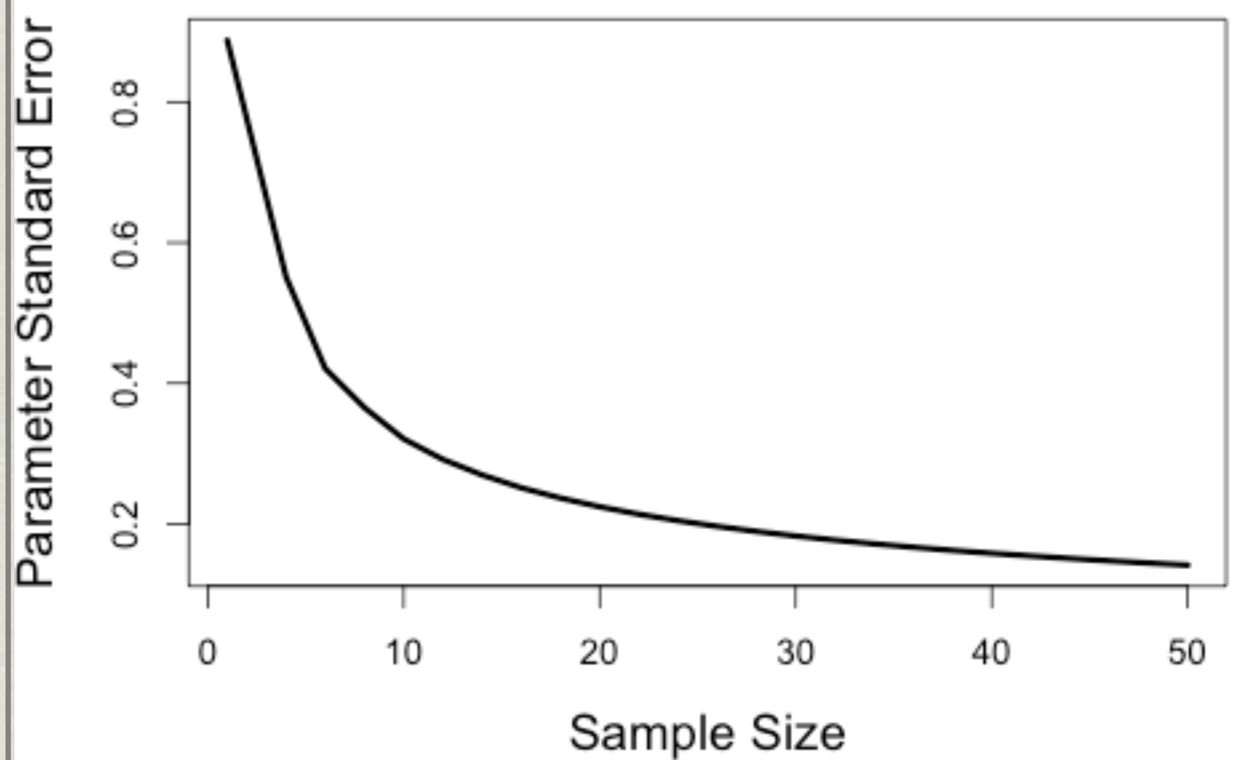
for(k in 1:M)

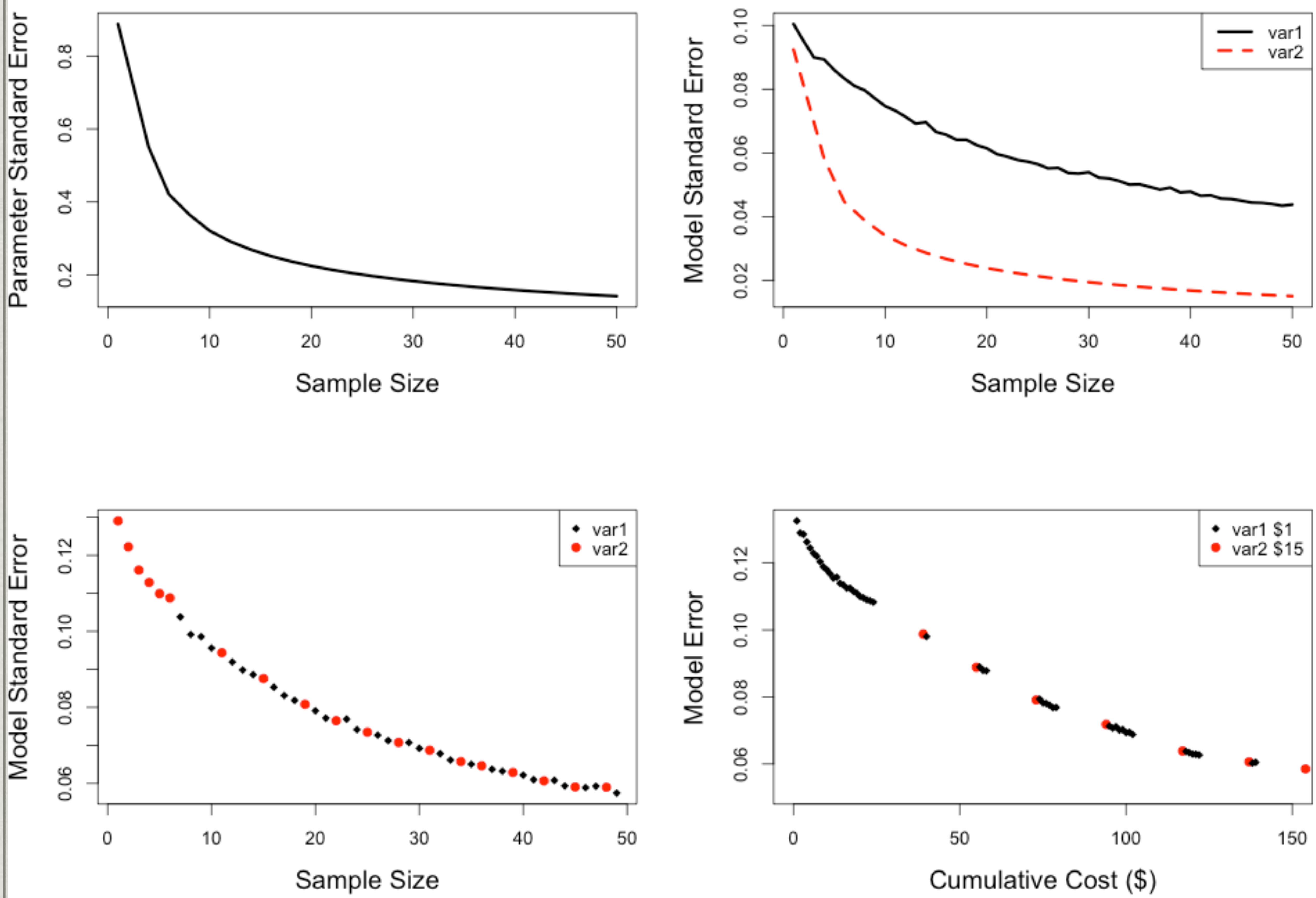
Draw random data of size N

Fit model

Save Parameters

- Nonparameteric bootstrap: resample data
- Parameteric bootstrap: assume param, sim data
- Embed in overall loop over N or different effect sizes
- Summarize distribution


Parameter Standard Error
0.2
0.4
0.6
0.8
0
10
20
30
40
50
Sample Size

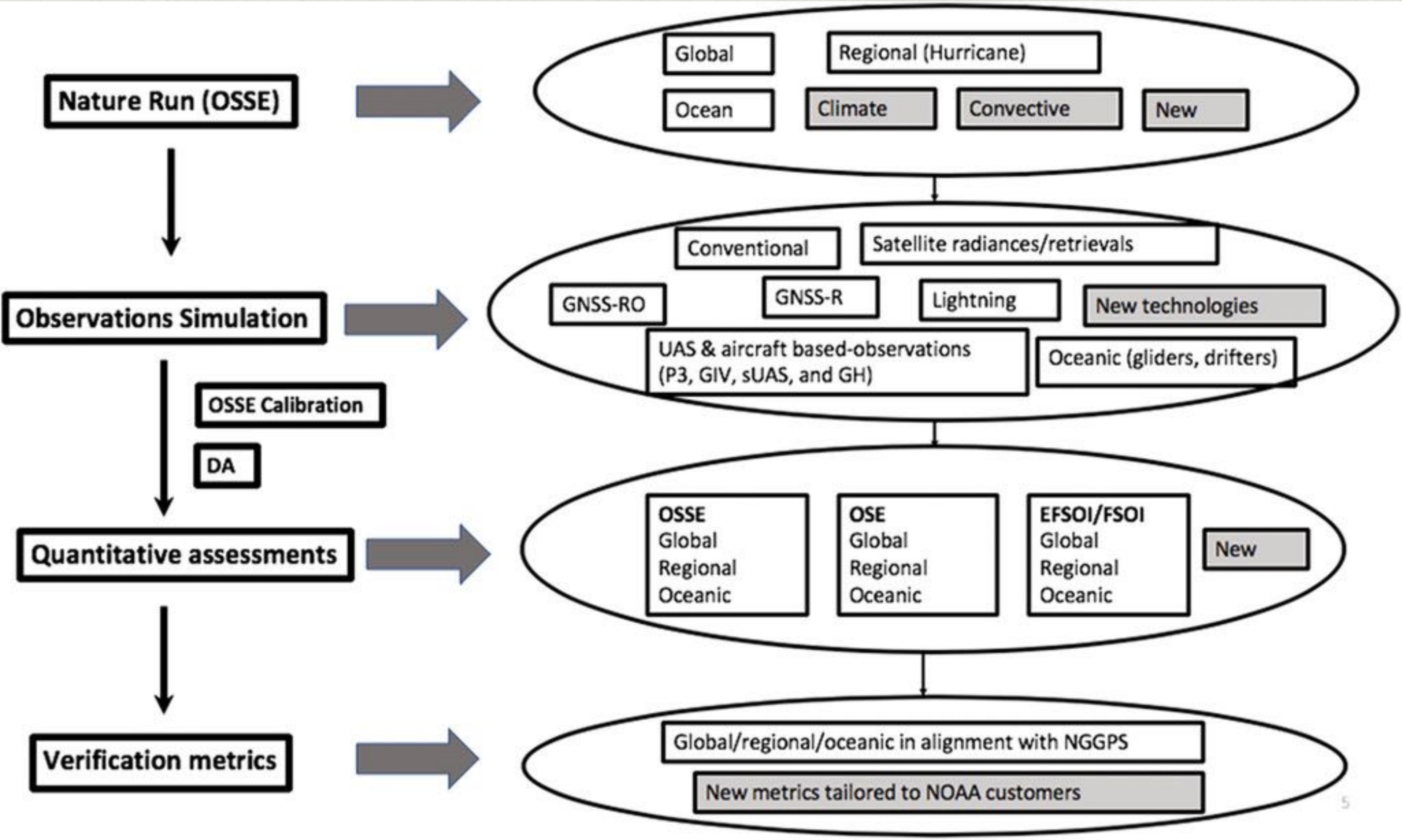


Parameter Standard Error
0.2
0.4
0.6
0.8
0
10
20
30
40
50
Sample Size
Model Standard Error
0.02
0.04
0.06
0.08
0.10
var1
var2
Sample Size
Model Standard Error
0.06
0.08
0.10
0.12
var1
var2
Sample Size
Model Error
var1 $1
var2 $15
0
50
100
150
Cumulative Cost ($)

Observing System Simulation Experiments

- Simulate “true” system
- Simulate pseudo-observations
- Assimilate pseudo-observations
- Assess impact on estimates

- **Augment an existing network**
  - **Additional locations**
  - **New Sensors**
- **Common in Weather, Remote Sensing, Oceanography**



Zeng et al 2020 "Use of Observing System Simulation Experiments in the United States" BAMS https://doi.org/10.1175/BAMS-D-19-0155.1